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Predicting Polarized Light Scattering by Marine Micro-Organisms

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Research Goals

To understand and quantify light scattering from ensembles of irregularly-shaped objects. To characterize the effect of ensembles of micro-organisms on the propagation of polarized light through sea water. To determine the feasibility of detecting particle orientation and to assess the importance of scattering to underwater imaging techniques and irradiance calculations.

Objectives

To develop a numerical or analytical model that predicts angle-dependent scattering of polarized light from ensembles of non-spherical marine organisms and marine detritus. To verify and examine the validity and range of applications of the model by comparison with exact calculations and/or experimental results as appropriate. Specific tasks toward the objectives are: (1) to develop an artificial neural network to recognize features in the scattering matrix elements associated with the irregular shape of oceanic scatterers, and (2) to refine and enhance the coupled-dipole approximation method.

Approach

The polarization states of the incident and scattered light are described by four-element Stokes vectors and the effect of the scattering medium on the incident beam is described by the sixteen-element Mueller or scattering matrix. Light scattering by spherical particles is determined by Mie calculations. For irregularly-shaped particles, the components of the scattered electric field are calculated using the coupled-dipole (C-D) approximation model. In this model, an arbitrarily-shaped object is divided into a number of identical dipolar oscillators arranged on a cubic lattice. Interactions between dipoles are included by determining the field at a particular dipole due to the incident field and the fields induced by the other dipole oscillators. The scattered field is the sum of the fields due to each oscillator. The Mueller matrix elements are calculated from the components of the scattered field. A numerical average of the Mueller matrix elements over a set of orientations of a single particle is accomplished by fixing the particle and rotating the coordinate axes

through the Euler angles. All computations using the coupled-dipole model are carried the Naval Oceanography Program's Cray Y-MP8.

An artificial neural net model is developed to analyze the scattering from spherical and non-spherical particles. The extensive analysis of Hunt and Quinby-Hunt in comparing the results of calculations using Mie theory with experimental measurements of the angular-dependent Mueller matrix elements for marine *Chlorella* serves as a standard to test the capability of the neural network.

Tasks Completed

The development of computer codes for calculating the sixteen elements of the Mueller scattering matrix for a collection of randomly oriented particles was completed during the last reporting period. Gaussian-Legendre integration over Euler angles was rigorously tested and proved to be a reliable method for calculating an orientational average of the Mueller matrix elements. Extensive calculations were made with the enhanced C-D model for collections of particles of various shapes including cylinders, cubes, prolate spheroids, hexagonal disks and helices. Spherical particles were also modeled so that comparisons could be made with Mie theory to assess limitations and ranges of application for the C-D calculations.

Although not yet completed, work is underway on the design and training of an artificial neural network to analyze light scattering from spherical and non-spherical particles. We hope to train the neural net to recognize features that are peculiar to scattering from irregularly-shaped particles. Limited success has been achieved with the neural net, but the results do show some promise. A problem with the neural net approach is the need for large amounts of data for training the network.

During the summer of 1994, the Principal Investigator and an undergraduate student worked with Arlon Hunt and Mary Quinby-Hunt at Lawrence Berkeley Laboratory. They began work on nebulizer system to produce aerosols similar to those found in the marine boundary layer. Mueller matrix elements for the light scattered by these aerosols were measured using the polarization-modulated nephelometer developed by Arlon Hunt.

Scientific Results

The good agreement of the coupled-dipole calculations with both the Mie theory (Figure 1) and the experimental data (Figure 2) for light scattering from spheres at size parameters around five and possibly larger is promising. A size parameter of six translates into a particle size in the ocean of about one micrometer at visible light wavelengths. Many marine organisms and particulates of interest have sizes between one and two micrometers, putting them within, or close, to the current modeling limits of the coupled-dipole method. Differences between coupled-dipole and Mie calculations at large scattering angles indicates that the coupled-dipole

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model should be used with caution for scattering of visible light from irregularly-shaped particles much larger than one micron. The model could be employed, however, to predict trends or prominent features in the scattering. The comparisons between the experimental measurements of the scattering matrix elements of bacteria spores and the calculated values for similarly-shaped ellipsoids using the CD-approximation are shown in Figures 3 and 4. Although the comparisons are not good, some trends are evident. It is likely that the failure to obtain better agreement between the bacteria spores and the ellipsoids is due to the compolex internal structure of the bacteria spore instead of its general shape.

The results of the comparison we have made between spheres (Mie Calculations) and ellipsoids (C-D calculations) of various aspect ratios provide an understanding of the degree to which non-spherical particles in the scattering medium effect the polarization state of the scattered light. (See Figure 5) In addition to this understanding, the results can also serve as a guide for determining when Mie calculations are adequate to describe scattering from a collection of particles and when we must use a model that includes scattering from non-spherical particles.

Mie calculations can provide adequate data for training a neural network to recognize spheres of varying size parameters and relative indices of refraction, but considerably more data is required to train the network to recognize features associated with non-spherical particles. Until additional data can be generated with the coupled-dipole approximation or when experimental data becomes available for non-spherical particles, an artificial neural network cannot be properly trained and evaluated. For this reason, future plans for this project include an experimental component at TSU to supplement the experimental work of Hunt and Quinby-Hunt at LBL.

Accomplishments

We have made considerable progress toward developing a practical model of polarized light scattering from non-spherical particles. Mueller matrix elements for single particles and collections of randomly oriented spheres, helices, cubes, ellipsoids and cylinders calculated with the C-D approximation have been compared with experimental measurements and with Mie calculations. Since Mie calculations have been shown to accurately predict the scattering for marine organisms that are nearly spherical, comparisons of the results of Mie calculations with those obtained for irregularly-shaped particles using the C-D method helps to establish the limits of applicability of the Mie theory to non-spherical particles.

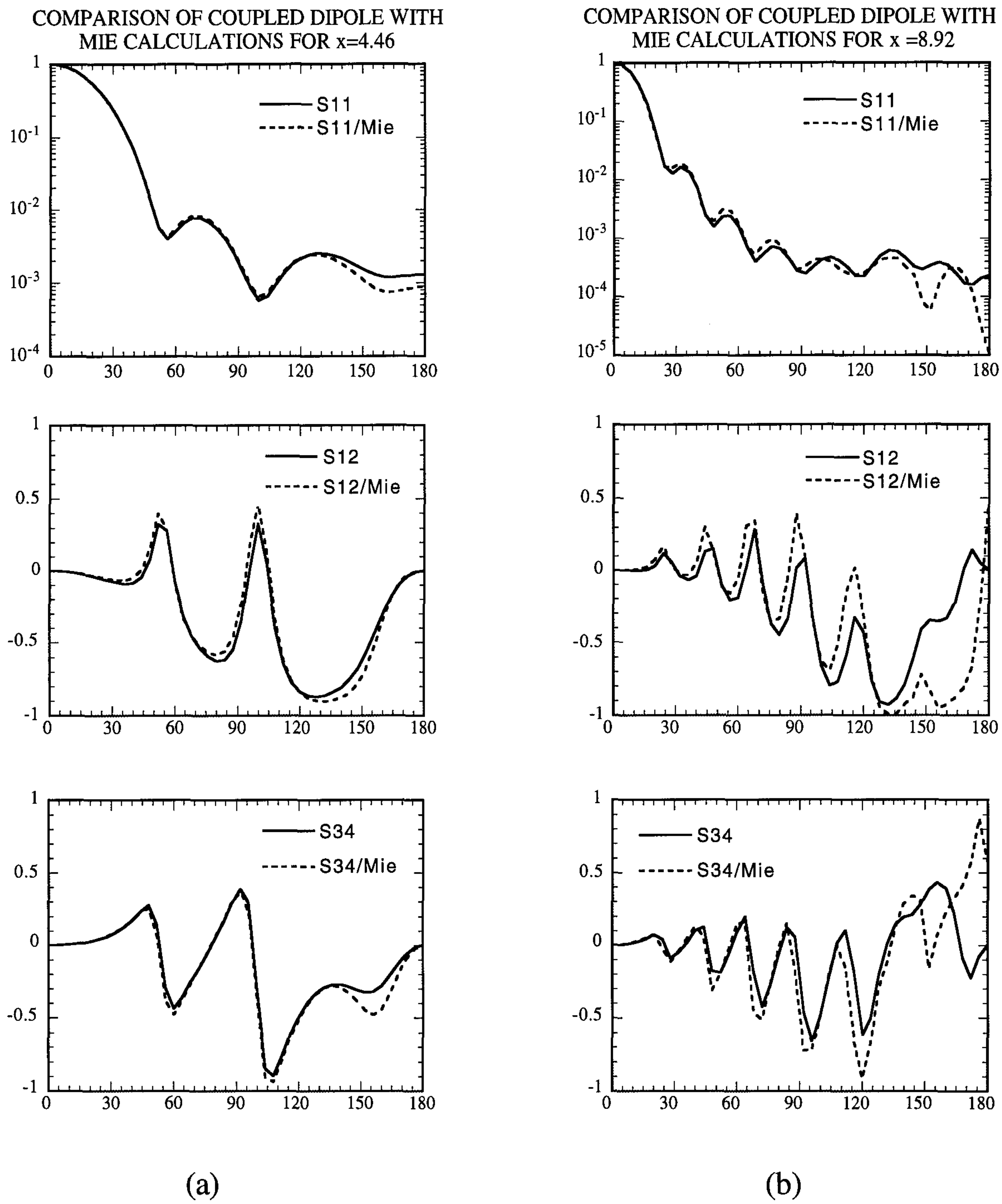

Figure 1. Comparison of the Mie calculations and the coupled-dipole approximation for spheres. The solid line represents coupled-dipole theory and dashed line represents Mie theory. Spheres with a size parameter of 4.46 are shown in column (a) and spheres with a size parameter of 8.92 are shown in column (b). In the coupled-dipole approximation, the sphere is modeled with 925 dipoles. In both calculations, the wavelength of incident light is 442 nm in air, the index of refraction of the medium (water) is 1.33, and the index of refraction of the sphere is 1.596.

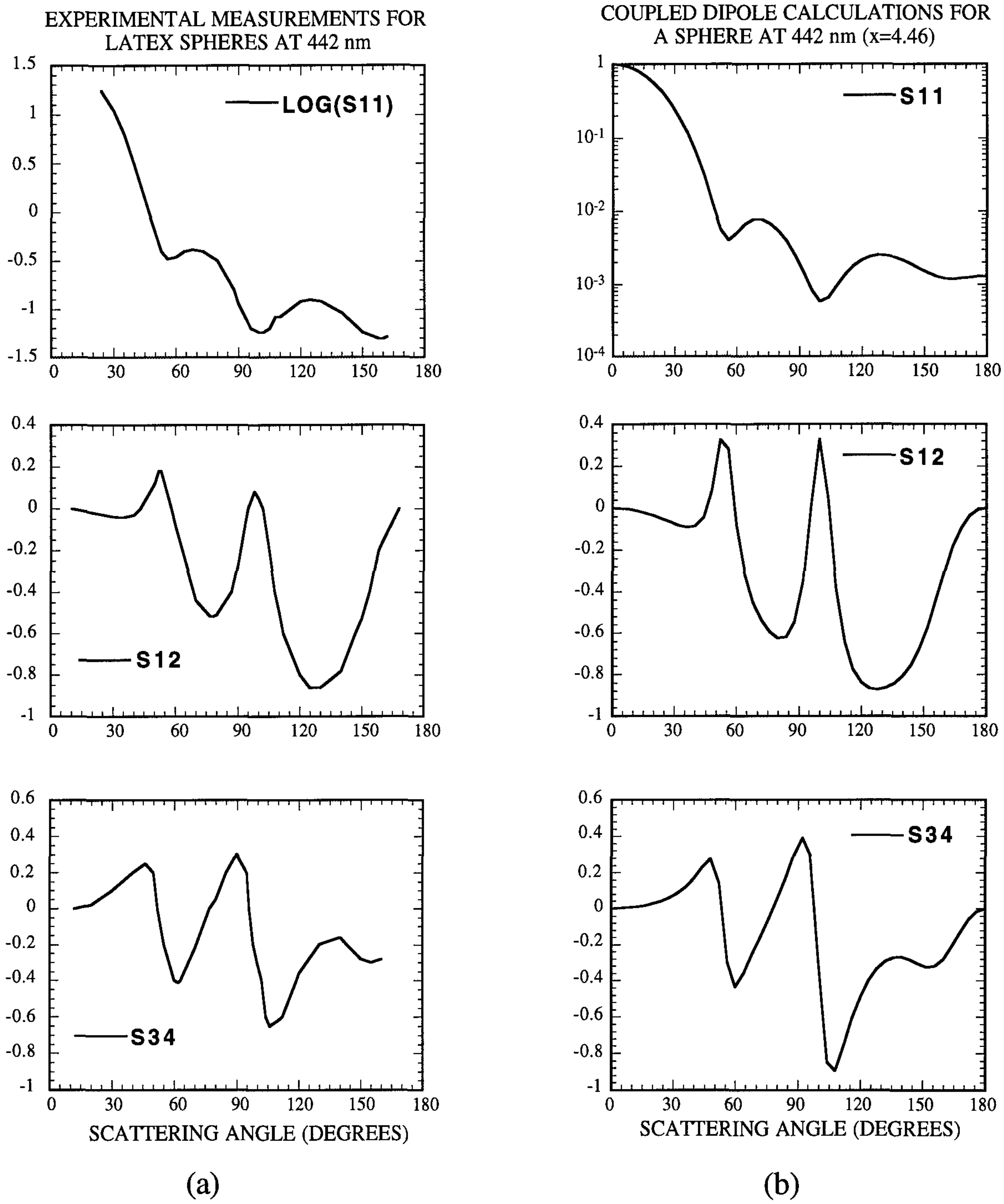

Figure 2. (a) Experimental measurements of the Mueller matrix elements for latex spheres. (b) Coupled-dipole calculations of the corresponding matrix elements for spheres of equivalent size parameter. In the coupled-dipole calculation, the sphere is modeled with 925 dipoles. In both figure, the wavelength of the incident light is 442 nm in air. The index of refraction of the medium (water) is 1.33 and the index of refraction of the sphere is 1.596.

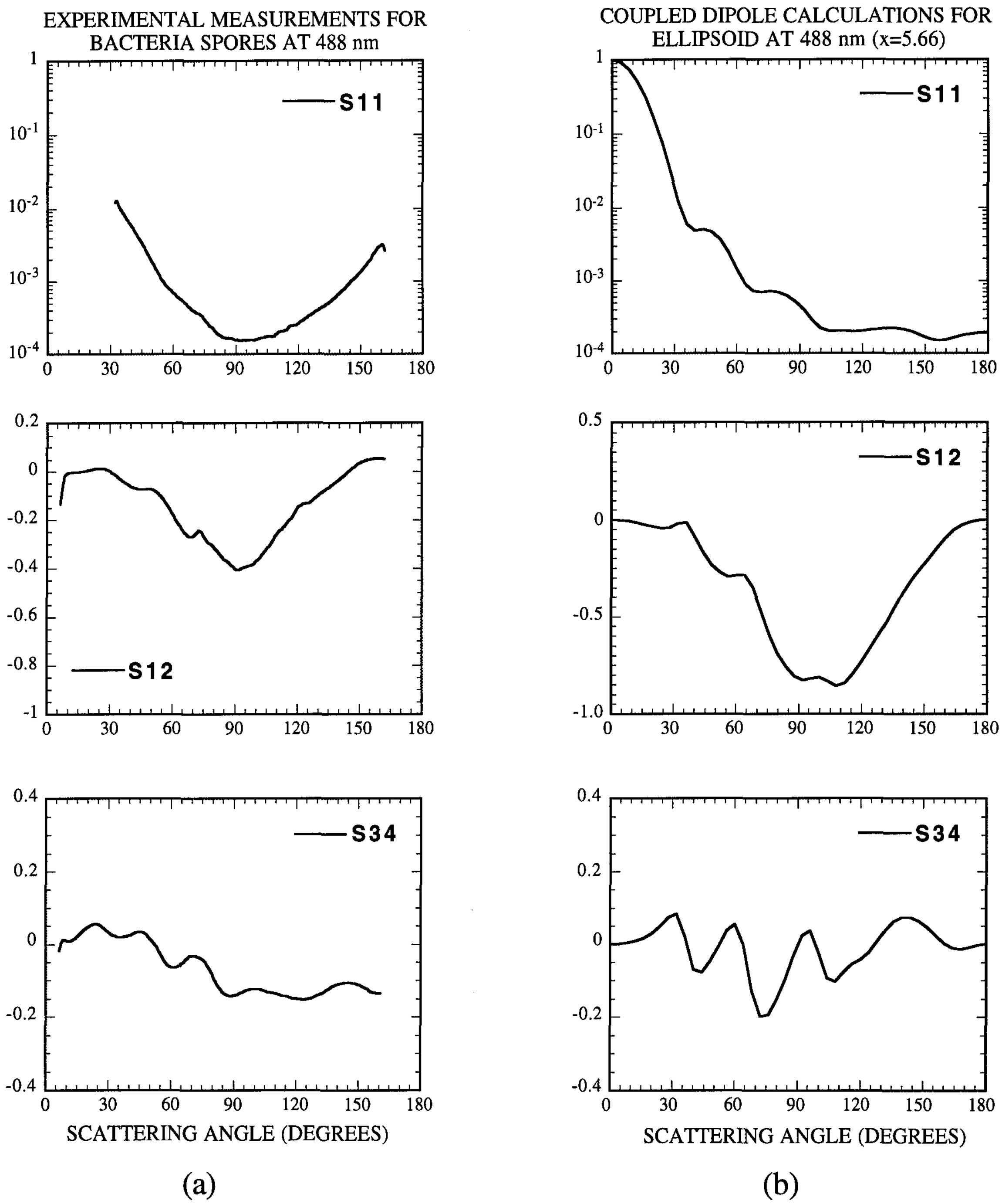

Figure 3. (a) Experimental measurements of the Mueller matrix elements for the *B. subtilus* spores. (b) Coupled-dipole calculations of the corresponding matrix elements for an ellipsoid. In the coupled-dipole calculations, the ellipsoid is modeled by 1032 dipoles and has a ratio of major to minor axis of 2.0. In both figures, the wavelength of incident light is 488 nm in air, the index of refraction of the medium (water) is 1.33 and the index of refraction of the ellipsoid is 1.48.

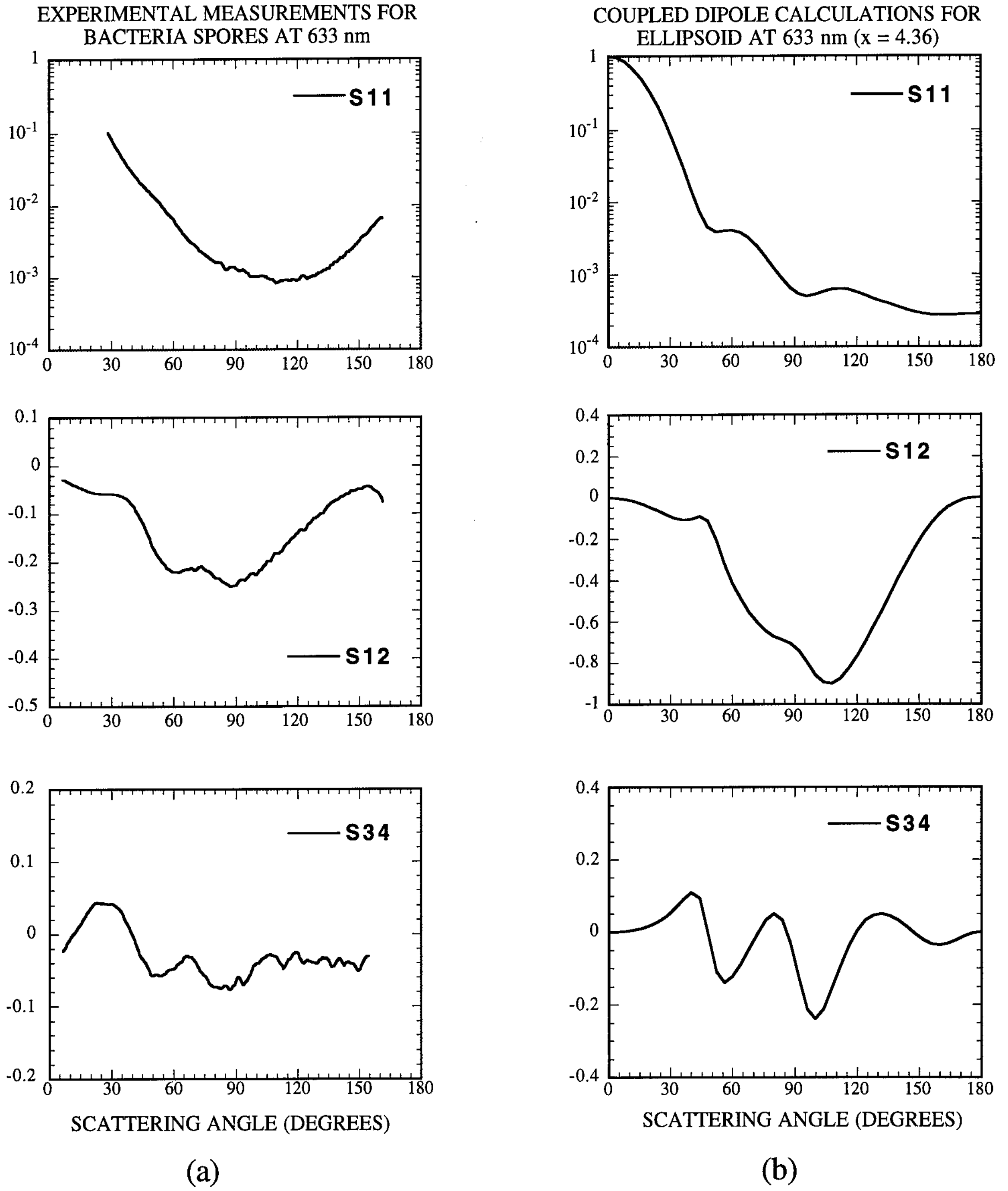

Figure 4. (a) Experimental measurements of the Mueller matrix elements for the *B. subtillus* spores. (b) Coupled-dipole calculations of the corresponding matrix elements for an ellipsoid. In the coupled-dipole calculations, the ellipsoid is modeled by 1032 dipoles and has a ratio of major to minor axis of 2.0. In both figures, the wavelength of incident light is 633 nm in air, the index of refraction of the medium (water) is 1.33 and the index of refraction of the ellipsoid is 1.48.

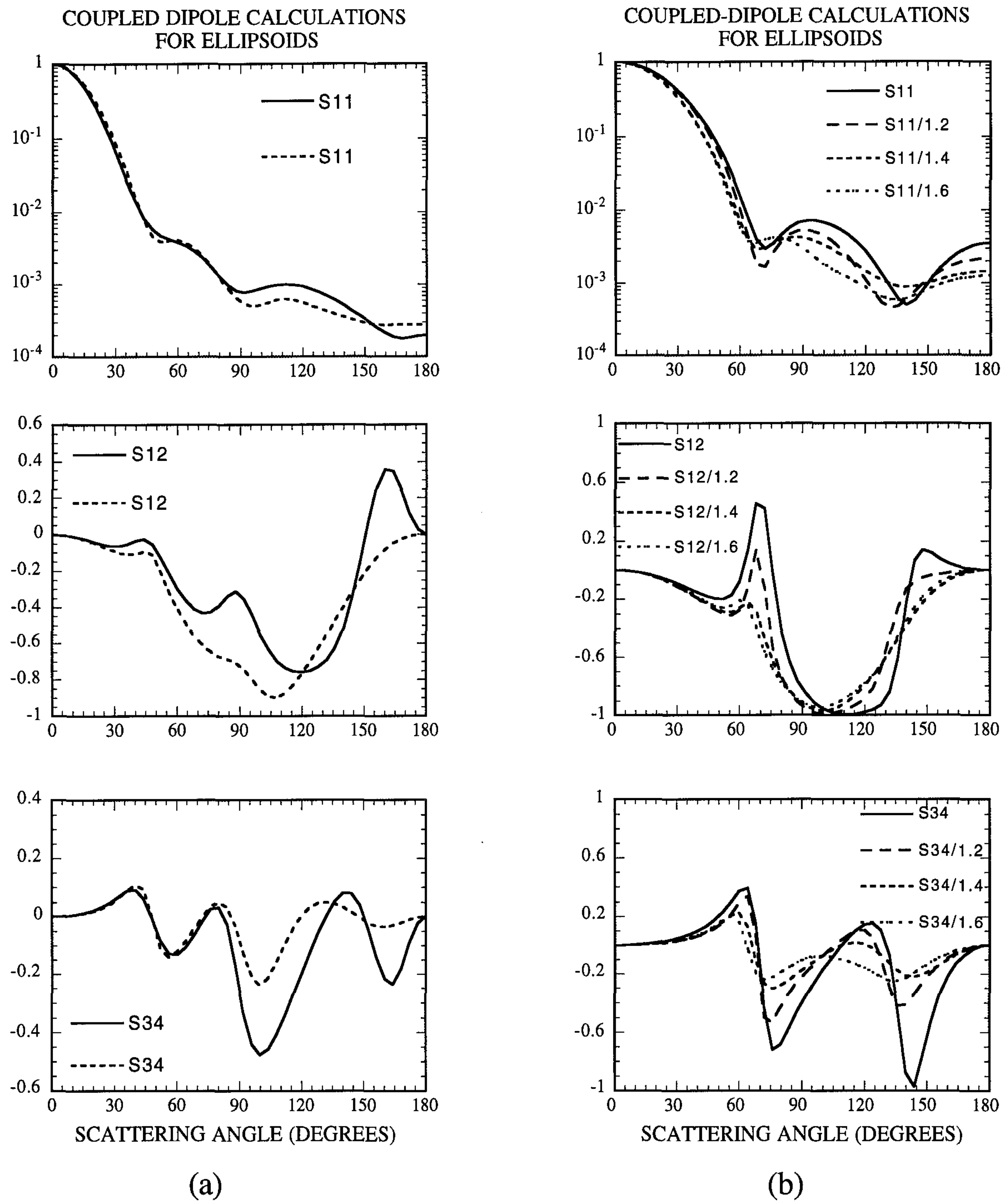

Figure 5. (a) Coupled-dipole calculations of the Mueller matrix elements for ellipsoids of two different values of the relative index of refraction. The solid line represents an ellipsoid with a relative index of refraction of 1.19 and the dashed line a relative index of refraction of 1.11. The size parameters are kept constant at 4.36 for both values of the relative index of refraction. (b) Mueller matrix elements for ellipsoids of varying ratios of major to minor axis. The solid line represents a sphere. Ratios of 1.2, 1.4 and 1.6 are labeled on each graph.

ONR-Sponsored Publications / Technical Reports

Shapiro, D.B., Quinby-Hunt, M.S., Hull, P.G., Hearst, J.E. and Hunt, A.J., 1994: Light scattering from marine dinoflagellates: single particle systems and ensembles, submitted to Special Section in Ocean Optics, Journal of Geophysical Research.

Shapiro, D.B., Hull, P.G., Hearst, J.E., and Hunt, A.J., 1994: Calculations of the Mueller scattering matrix for a DNA Plectonemic Helix, *J. Chem. Phys.*, Vol. **101** (5), 4214-4221.

Shapiro, D.B., Hull, P.G., Hunt, A.J., Shi, Y., McClain, M.F., Quinby-Hunt, M.S., Hearst, J.E., 1994: Determination of the Average Orientation of DNA in the Octopus Sperm, *Eledone cirrhosa* using Polarized Light Scattering, *Appl. Opt.* Vol. **33**, 5733-5744.

Shapiro, D.B., Hull, P.G., Hunt, A.J., Shi, Y., Maestre, M.F., 1994: Quinby-Hunt, M.S., Hearst, J.E. Towards a working theory of polarized light scattering from helices, *J. Chem. Phys*. Vol. **100** (1), 146-157.

Hull, P., Shaw, F., Quinby-Hunt, M., Shapiro, Hunt, A. and Leighton, T. 1994: Comparison of analytical calculations with experimental measurements for polarized light scattering by marine micro-organisms," *Ocean Optics XII, Proc. SPIE,* Vol. **2258**.

Quinby-Hunt, M, Hull, P., Miller, D. and Hunt, An. 1994: Predicting polarization properties of marine aerosols, *Ocean Optics XII, Proc. SPIE,* Vol. **2258**.

STATISTICS

3 Papers published, referred journals
1 Papers submitted, refereed journals
0 Books or chapters published, refereed publication
0 Books or chapters submitted, refereed publication
0 Invited presentations
0 Contributed presentations
2 Technical reports and papers, non-refereed journals
3 Undergraduate students supported
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EEO/MINORITY SUPPORT

0 Female grad students
0 Minority grad students
0 Asian grad students
0 Female post-docs
0 Minority post-docs
0 Asian post-docs

Patents and awards 0

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